

Thermodynamics and transport in mesoscopic disordered networks

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Abstract

We describe the effects of phase coherence on transport and thermodynamic properties of a disordered conducting network. In analogy with weak-localization correction, we calculate the phase coherence contribution to the magnetic response of mesoscopic metallic isolated networks. It is related to the return probability for a diffusive particle on the corresponding network. By solving the diffusion equation on various types of networks, including a ring with arms, an infinite square network or a chain of connected rings, we deduce the magnetic response. As it is the case for transport properties –weak-localization corrections or universal conductance fluctuations– the magnetic response can be written in term of a single function S called spectral function which is related to the *spatial average* of the return probability on the network. We have found that the magnetization of an ensemble of **connected** rings is of the same order of magnitude as if the rings were disconnected.

I. INTRODUCTION

The understanding of persistent currents in mesoscopic rings is still an open problem since no quantitative agreement has yet been reached between theoretical developments and experimental results [Buttiker et al. 1983, Levy et al. 1990, Chandrasekhar et al. 1991, Mailly et al. 1993, Reulet et al. 1995, Mohanty et al. 1996, Montambaux 1996]. The only quantitative calculations of persistent currents relevant to the experimental situations rely on analytical methods in which disorder and interactions are treated perturbatively [Cheung et al. 1989, Ambegaokar et al. 1990, Schmid 1995, Von Oppen et al. 1991, Altshuler et al. 1991, Akkermans et al. 1991, Oh et al. 1991, Argaman et al. 1993, Argaman et al. 1993, Montambaux 1996]. The disorder is described in the usual framework of perturbation theory and interactions are treated in a Hartree-Fock approximation.

In ring experiments, the important parameters are certainly the strength of disorder and the strength of interactions. Both parameters are difficult to vary experimentally in a controlled way. In order to go beyond this problem, we have recently proposed to extend the analytical method to describe new geometries which generalize the ring topology, and which allow the variation of some geometric parameters in order to change the amplitude of the persistent current [Pascaud et al. 1997]. In the experiment done on a single Ga-As ring, for example, the ring was connected to leads [Mailly et al. 1993] and one may wonder how the current is changed when the lengths of the leads increase. On the other hand, experiments on many rings have been performed on an ensemble of *disconnected* rings [Levy et al. 1990, Reulet et al. 1995]. One may wonder whether the same effect persists when the rings are *connected*, i.e. what is the magnetization of a lattice, resulting from phase coherence.

Such a generalization, from the ring geometry to a network, had already been considered in the past to describe the weak-localization correction to the conductivity. This correction is related to the return probability, solution of a diffusion equation [Khmel'nitskii 1984]. This return probability has two components, a purely classical one and an interference term which results from interferences between pairs of time-reversed trajectories. In the diagrammatic picture, they are related to the diffuson and Cooperon diagrams. The interference term, $p_\gamma(\mathbf{r}, \mathbf{r}', \omega)$, is field dependent and is solution of the diffusion equation:

$$[\gamma - i\omega - D(\nabla + \frac{2ie\mathbf{A}}{\hbar c})^2]p_\gamma(\mathbf{r}, \mathbf{r}', \omega) = \delta(\mathbf{r} - \mathbf{r}') \quad (1)$$

where D is the diffusion coefficient. The scattering rate $\gamma = D/L_\phi^2$ describes the breaking of phase coherence. L_ϕ is the phase coherence length. γ will be compared to $1/\tau_D = D/L^2$ where τ_D is the diffusion time, typical time to diffuse through the system of size L . This time is the inverse of the Thouless energy. The classical probability obeys the same equation as (1) with $\mathbf{A} = 0$. By solving the diffusion equation (1) on various lattices, the weak-localization

correction was calculated by Douçot and Rammal [Doucot et al. 1986]. The persistent current of a ring, or in a more general geometry the mesoscopic magnetization, have a different nature. They are thermodynamic and not transport quantities. Transport properties exhibit weak-localization effects because they are response functions related to the propagation of two states: the conductivity is written in terms of a product of two Green functions whose disorder average is related to the return probability. A priori, average thermodynamic quantities do not exhibit weak-localization corrections since they are integrals of the density of states, i.e. they are written in terms of a single Green function. This is why the average persistent current $\langle I \rangle$ of non interacting electrons vanishes for an ensemble of rings. However, the typical current, $I_{typ} = \sqrt{\langle I^2 \rangle}$ involves the product of two propagators. Similarly, the average Hartree-Fock correction to the average current does not vanish because the interaction term also contains two propagators. As a result, these quantities are expected to be related to weak-localization effects and to the return probability.

This paper is organized as follows: in the next section, we recall how to solve the diffusion equation on a lattice and we calculate the weak-localization correction. In section III, the persistent current and the mesoscopic magnetization are related to the return probability and are calculated for a few geometries in section IV. In the last section, we show how the universal conductance fluctuations are related to the return probability and we calculate them for the simple geometry of the single wire, using this simple approach.

II. DIFFUSION ON A LATTICE - WEAK-LOCALIZATION CORRECTION

Let us first recall that the weak-localization correction to the conductance of a connected mesoscopic sample can be written in term of the interference part of the return probability [Khmelnitskii 1984, Doucot et al. 1986]:

$$\Delta\sigma(r) = -2s(e^2/h)DC_\gamma(\mathbf{r}, \mathbf{r}) \quad (2)$$

s is the spin degeneracy. The Cooperon $C_\gamma(\mathbf{r}, \mathbf{r}, H)$ is the time integrated field-dependent return probability: $C_\gamma(\mathbf{r}, \mathbf{r}, H) = \int_0^\infty p_\gamma(\mathbf{r}, \mathbf{r}, t, H)dt = p_\gamma(\mathbf{r}, \mathbf{r}, \omega = 0, H)$. Douçot and Rammal [Doucot et al. 1986] have calculated the weak-localization corrections on various networks. Considering networks made of quasi-1D wires, so that the diffusion can be described as one-dimensional, the Cooperon $C_\gamma(r, r')$ obeys the one-dimensional diffusion equation

$$[\gamma - D(\nabla + \frac{2ieA}{\hbar c})^2]C_\gamma(r, r') = \delta(r - r') \quad (3)$$

with the continuity equations written for every node α (including the starting point r' that can be considered as an additional node in the lattice) [Doucot et al. 1986]

$$\sum_\beta (-i\frac{\partial}{\partial r} + \frac{2eA}{\hbar c})C_\gamma(r, r')|_{r=\alpha} = \frac{i}{DS}\delta_{r',\alpha} \quad (4)$$

r, r' are linear coordinates on the network. The sum is taken over all links relating the node α to its neighboring nodes β . Integration of the differential equation (3) with the boundary conditions (4) leads to the so-called network equations which relate $C_\gamma(\alpha, r')$ to the neighboring $C_\gamma(\beta, r')$.

$$\sum_{\beta} \coth\left(\frac{l_{\alpha\beta}}{L_\phi}\right) C(\alpha, r') - \sum_{\beta} \frac{C(\beta, r') e^{-i\gamma_{\alpha\beta}}}{\sinh(l_{\alpha\beta}/L_\phi)} = \frac{L_\phi}{DS} \delta_{\alpha, r'} \quad (5)$$

$l_{\alpha\beta}$ is the length of the link $(\alpha\beta)$ and $\gamma_{\alpha\beta} = (4\pi/\phi_0) \int_{\alpha}^{\beta} \mathbf{A} d\mathbf{l}$ is the circulation of the vector potential along this link. Solving this set of linear equations and performing the spatial integration of $C_\gamma(r', r')$ give access to the weak-localization correction.

III. PERSISTENT CURRENTS AND MESOSCOPIC MAGNETIZATION

The magnetization $M(H)$ is the derivative of the free energy F with respect to the magnetic field H : $M = -\frac{\partial F}{\partial H}$. Introducing the field dependent DOS (for one spin direction), $\rho(\epsilon, H)$, the magnetization is written at zero temperature as (taking the spin into account):

$$M = -2 \frac{\partial}{\partial H} \int_{-\epsilon_F}^0 \epsilon \rho(\epsilon, H) d\epsilon \quad (6)$$

The origin of energies is taken at the Fermi energy. The average magnetization is thus related to the field dependence of the average density of states $\langle \rho(\epsilon, H) \rangle$. In a bulk system, this leads to the Landau diamagnetism. In the thin ring geometry where no field penetrates the conductor, the DOS only depends on the Aharonov-Bohm flux. Its average is flux independent because the flux modifies only the phase factors of the propagator which cancel in average. During the last years, there has been a large amount of work to explain the origin of a non-zero average current, as observed experimentally. The constraint that the number of particles is fixed in each ring leads to an additional contribution to the average current often referred as the "canonical" current [Bouchiat et al. 1989, Imry 1991]. Its amplitude is however very small [Schmid 1995, Von Oppen et al. 1991, Altshuler et al. 1991, Akkermans et al. 1991]. As we will see later, a larger contribution comes from the effect of interactions.

We first calculate the typical magnetization M_{typ} , defined as $M_{typ}^2 = \langle M^2 \rangle - \langle M \rangle^2$. From eq.(6), it can be written as:

$$M_{typ}^2 = 4 \frac{\partial}{\partial H} \frac{\partial}{\partial H'} \int_{-\epsilon_F}^0 \int_{-\epsilon_F}^0 \epsilon \epsilon' K(\epsilon - \epsilon', H, H') d\epsilon d\epsilon' \quad (7)$$

where K is the correlation function of the DOS: $K(\epsilon - \epsilon', H, H') = \langle \rho(\epsilon, H) \rho(\epsilon', H') \rangle - \rho_0^2$. $K(\epsilon)$ has been calculated by Altshuler and Shklovskii [Altshuler et al. 1986] for a bulk system and later in the presence of a magnetic flux [Schmid 1995, Von Oppen et al. 1991, Altshuler et al. 1991, Akkermans et al. 1991] for the ring geometry. A very useful semiclassical

picture has been presented by Argaman *et al.*, which relates the form factor $\tilde{K}(t)$, the Fourier transform of $K(\varepsilon)$, to the integrated return probability $P(t) = \int p(\mathbf{r}, \mathbf{r}, t) d\mathbf{r}$ for a diffusive particle [Argaman et al. 1993]:

$$\tilde{K}(t) = tP(t)/(4\pi^2) \quad (8)$$

In this picture, like the return probability, the form factor is the sum of a classical and an interference term:

$$\tilde{K}(t, H, H') = \frac{t}{4\pi^2} [P_\gamma(t, \frac{H-H'}{2}) + P_\gamma(t, \frac{H+H'}{2})] \quad (9)$$

Fourier transforming $K(\epsilon - \epsilon')$ and using the identity $\int_0^\infty \epsilon d\epsilon e^{i\epsilon t} = -1/t^2$, one obtains straightforwardly¹:

$$M_{typ}^2(H) = \frac{1}{2\pi^2} \int_0^\infty \frac{P_\gamma''(t, H)|_0^H}{t^3} dt, \quad (10)$$

where $P_\gamma''(t, H)|_0^H = \partial^2 P_\gamma / \partial H^2|_H - \partial^2 P_\gamma / \partial H^2|_0$.

We now turn to the average magnetization. It has been found that the Hartree-Fock(HF) correction to the energy leads to an average persistent current in a ring [Ambegaokar et al. 1990, Schmid 1995]. The average magnetization can be written as [Argaman et al. 1993, Montambaux 1996]:

$$\langle M_{ee} \rangle = -\langle \frac{\partial E_T}{\partial H} \rangle = -\frac{U}{4} \frac{\partial}{\partial H} \int \langle n^2(\mathbf{r}) \rangle d\mathbf{r} \quad (11)$$

where the screened Coulomb interaction is $U = 4\pi e^2/q_{TF}^2$ [Eckern 1991]. q_{TF} is the Thomas-Fermi vector. The magnetization can be rewritten in terms of the two-point correlation function of the local density of states and then in term of the return probability [Montambaux 1996]:

$$\langle M_{ee} \rangle = -\frac{U\rho_0}{\pi} \frac{\partial}{\partial H} \int_0^\infty \frac{P_\gamma(t, H)}{t^2} dt \quad (12)$$

It appears that $\langle M_{ee} \rangle$ and $\langle M_{typ} \rangle$ are time integrals of the return probability with various power-law weighting functions. Noting that $P_\gamma(t)$ has the form $P_0(t)e^{-\gamma t}$, all these quantities

¹The lower bound of the time integrals is actually the mean collision time τ_e above which diffusion takes place.

can be written as integrals of a single function $S(\gamma, H)$ that we call the spectral function²

$$S(\gamma, H) = \int \frac{P_0(t, H)}{t} e^{-\gamma t} dt = \int_{\gamma}^{\infty} d\gamma \int C_{\gamma}(\mathbf{r}, \mathbf{r}, H) d\mathbf{r} \quad (13)$$

The different magnetizations can be given in terms of the successive integrals of this function:

$$\langle M_{ee}(H) \rangle = -\frac{U\rho_0}{\pi} \frac{\partial}{\partial H} S^{(1)}(\gamma, H) \quad (14)$$

$$M_{typ}^2(H) = \frac{1}{2\pi^2} \frac{\partial^2}{\partial H^2} S^{(2)}(\gamma, H)|_0^H \quad (15)$$

where $S^{(n)}(\gamma) = \int_{\gamma}^{\infty} d\gamma_n \dots \int_{\gamma_2}^{\infty} d\gamma_1 S(\gamma_1)$.

IV. EXAMPLES

We first consider the case of a ring of perimeter L connected to one arm of length b , see fig.1. Such a geometry has been considered in the strictly 1D case without disorder [Buttiker 1985, Buttiker 1994, Akkermans et al. 1991, Mello 1993]. It is expected that since the electrons will spend some time in the arm where there are not sensitive to the flux, the magnetization will be decreased. From eqs. (3,5), the function $C_{\gamma}(r, r, H)$ can be straightforwardly calculated on the arm and on the ring. Spatial integration gives:

$$S(\gamma, H) = -\ln\left[\frac{1}{2} \tanh \frac{b}{L_{\phi}} \sinh \frac{L}{L_{\phi}} + \cosh \frac{L}{L_{\phi}} - \cos 4\pi\varphi\right]$$

where $\varphi = \Phi/\phi_0$. Φ is the flux through the ring, $\phi_0 = h/e$ is the flux quantum. $\gamma\tau_D = (L/L_{\phi})^2$. $\langle M_{ee} \rangle$ and M_{typ} are given by successive integrations over γ according to eqs.(14,15). They can be compared to the case of a single loop without arm. We find that they decrease when b increases and saturate to a finite value when $b \gg L_{\phi}$. The m^{th} harmonics of the flux dependence of $\langle M_{ee} \rangle$ is smaller by a factor $(2/3)^m$ and the m^{th} harmonics of M_{typ} is smaller by a factor $(2/3)^{m/2}$.

In the case of a ring connected to two diametrically opposite infinitely long arms, fig.1, the m^{th} harmonics of $\langle M_{ee} \rangle$ is smaller by a factor $(4/9)^m$ and the reduction factor is $(2/3)^m$ for the typical magnetization. This result is relevant for the experiment of ref. [Mailly et al. 1993] where the magnetization is measured for open and connected rings. Moreover, in the limit

²This function S is related to the logarithm of the spectral determinant defined in ref. [Andreev et al. 1995]. The number variance for a closed system can be written as

$$\Sigma^2(E) = \frac{2s^2}{\beta\pi^2} \Re[S(\gamma) - S(\gamma + iE)]$$

where s is the spin degeneracy and $\beta = 1$ in zero field, $\beta = 2$ if time reversal symmetry is broken.

$b \gg L_\phi$, the magnetization should be unchanged if reservoirs are attached to the arms. We propose that single ring experiments with appropriately designed arms should be able to measure these reductions.

We now turn to the case of an infinite square lattice whose average magnetization will be compared with the one of an array of isolated rings. The eigenvalues of the diffusion equation can be calculated for a rational flux per plaquette $\varphi = Ha^2/\phi_0 = p/2q$. a is the lattice parameter. Defining $\eta = a/L_\phi$, we find that the spectral function $S(\gamma, H)$ is

$$S(\gamma, H) = -\frac{1}{q} \sum_{i=1}^q \langle \langle \ln(4 \cosh \eta - \varepsilon_i(\theta, \mu)) \rangle \rangle \quad (16)$$

where $\langle \langle (\dots) \rangle \rangle = \int_0^{2\pi} \frac{d\theta}{2\pi} \int_0^{2\pi} \frac{d\mu}{2\pi} (\dots)$. $\varepsilon_i(\theta, \mu)$ are the solutions of the determinantal equation $\det M = 0$ where the $q \times q$ matrix M is defined by $M_{nn} = 2 \cos(4n\pi\varphi + \theta/q) - \varepsilon$, $M_{n,n+1} = M_{n+1,n} = 1$ for $n \leq q-1$ and $M_{1,q} = M_{q,1}^* = \exp(i\mu)$. This is the matrix associated to the Harper equation known to be also relevant for other related problems like tight-binding electrons in a magnetic field [Hofstadter 1976] or superconducting networks in a field [Rammal et al. 1983].

The expression (16) can be compared to the spectral function for a square ring of perimeter $L = 4a$:

$$S(\gamma, H) = -\ln(\cosh 4\eta - \cos 4\pi\varphi) \quad (17)$$

From eq.(14), one calculates $\langle M_{ee} \rangle$:

$$\langle M_{ee} \rangle = U\rho_0 \frac{eD}{\pi^2 q} \frac{\partial}{\partial \varphi} \sum_{i=1}^q \int_{\eta}^{\infty} \{ \ln(4 \cosh \eta - \varepsilon_i(\theta, \mu)) \} \eta d\eta$$

which is a continuous and derivable function of the field. It can be compared with the ring magnetization which can be cast in the form:

$$\langle M_{ee} \rangle = U\rho_0 \frac{4eD}{\pi} \int_{\eta}^{\infty} \frac{\sin 4\pi\varphi}{\cosh 4\eta - \cos 4\pi\varphi} \eta d\eta \quad (18)$$

The magnetization density is plotted on fig.2 for the ring and the infinite lattice. It is seen that the network magnetization density is about 25 times smaller than the ring magnetization. Considering that on the array of square rings already considered experimentally [Levy et al. 1990, Reulet et al. 1995], the distance between rings is equal to the size of the squares, the number of squares is four times larger when they are connected. One then expects only a factor of order 6 between the magnetization of the array of disconnected rings and the lattice.

We have also calculated the magnetization of a chain of rings connected with arms of similar length, an obvious generalization of the experiment done in ref. [Mohanty et al. 1996] and we find that when the rings are connected the average Hartree-Fock magnetization is reduced by a factor 3.

In conclusion, we showed that persistent current experiments do not necessarily require the rings to be disconnected and we suggest to perform magnetization experiments on arrays of connected rings.

V. TRANSPORT

We now come back to the calculation of transport properties in term of the spectral function $S(\gamma)$, with application to the well-known case of an open wire as an example. From eq.(2), the dimensionless conductance $g = G/(e^2/h)$ is given by (for one spin direction):

$$\langle \delta g \rangle = -2 \int P(t) \frac{dt}{\tau_D}$$

where $\tau_D = L^2/D$ is the diffusion time, inverse of the Thouless energy. This correction is easily written as a function of $S(\gamma)$:

$$\langle \delta g \rangle = 2 \frac{1}{\tau_D} \frac{\partial}{\partial \gamma} = 2 \frac{\partial S}{\partial x}$$

where $x = \gamma \tau_D = (L/L_\varphi)^2$.

Similarly the conductance fluctuation can be found directly as a function of the diffusion probability $p(r, r', t)$ [Argaman 1996]. Then, using some properties of the diffusion propagator, it can be cast in the form, for one spin direction:

$$\langle \delta g^2 \rangle = 12 \int P(t) \frac{t dt}{\tau_D^2}$$

or

$$\langle \delta g^2 \rangle = 12 \frac{1}{\tau_D^2} \frac{\partial^2 S}{\partial \gamma^2} = 12 \frac{\partial^2 S}{\partial x^2}$$

In the example of an open wire, the spectral function S is found to be, considering the appropriate boundary conditions:

$$S(x) = -\ln \frac{\sinh \sqrt{x}}{\sqrt{x}}$$

from which the weak-localization correction and the variance of the conductance fluctuations is immediately found. In particular, in the limit of complete phase coherence $L_\varphi \gg L$, i.e. $x \rightarrow 0$, the expansion of the function $S(x)$:

$$S(x) \rightarrow -\frac{x}{6} + \frac{x^2}{180}$$

immediately leads to the known universal values:

$$\begin{aligned}\langle \delta g \rangle &= 2S'(0) = -1/3 \\ \langle \delta g^2 \rangle &= 12S''(0) = 2/15\end{aligned}$$

The variance should be multiplied by two when there is time reversal symmetry. When L_ϕ is finite, the variance of the fluctuations is simply related to the mean weak-localization correction:

$$\langle \delta g^2 \rangle = -6 \frac{\partial}{\partial x} \langle \delta g \rangle \tag{19}$$

In conclusion, we have written various thermodynamic and transport properties in term of a single function called spectral function, which is related to the spatial average of the return probability. We are thus able to calculate these physical properties for any type of network.

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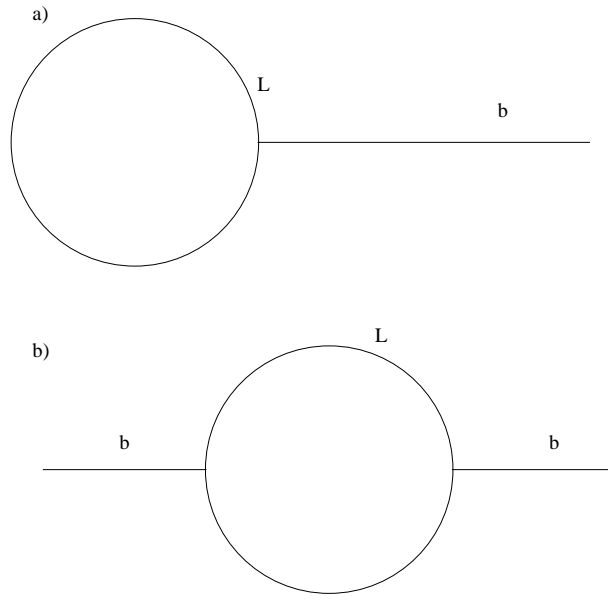


FIG. 1. Geometries of a ring with arms considered in the text

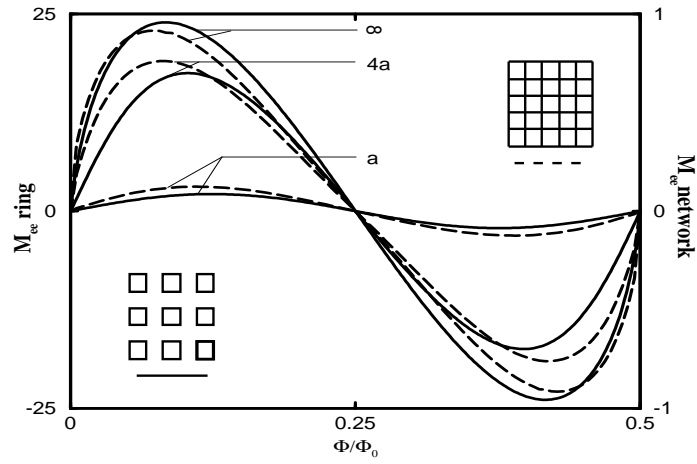


FIG. 2. Average magnetization $\langle M_{ee} \rangle$ of a single ring (full lines) and magnetization density of the infinite network (dashed lines), for $L_\phi = \infty$, $4a$ and a